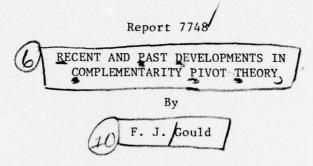
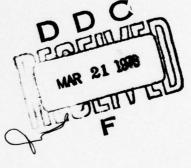


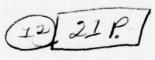
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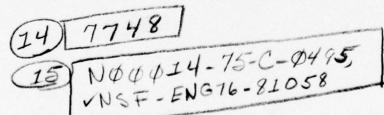
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RECENT AND PAST DEVELOPMENTS IN COMPLEMENTARY PIVOT THEORY 1

by

F. J. Gould²/ University of Chicago

1. <u>Introduction</u>. This year marks the end of the first decade of a stream of research launched by the appearance in 1967 of Herb Scarf's paper [33] on the approximation of fixed points of continuous maps via the technique of complementary pivoting. During this ten year period research has tended to emphasize simplicial approximation algorithms for finding fixed points, or, equivalently, zeros, of rather small but "highly nonlinear" systems. Contributions to this stream, in the way of algorithms and theoretic results, are due to, among others, Charnes, Garcia, and Lemke [4], Eaves [7], Eaves and Scarf [8], Fisher, Gould, and Tolle [10], Garcia and Gould [12], [13], [14], [15], Garcia and Zangwill [16], [17], Gould and Tolle [18], [19], Kuhn [22], [23], [24], Lemke [26], and Merrill [29]. The interested reader should also refer to the many additional authors referred to in the bibliographies of these works.

During this past ten years I would estimate that at least 100 publications on this topic have appeared either as papers in scholarly journals or as Ph.D. dissertations, and these have ranged from theoretic to computational studies. It thus seems clear that momentum is gathering in this area. The initial work

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of Scarf, along with the even earlier underlying work of Carl Lemke, has mushroomed into a prominent and quite active specialization in mathematical programming.

I should like to very briefly summarize only a few of the many past developments—in particular two with which I am most familiar. And then I will discuss three of what I consider to be the most exciting very recent developments. In order, the topics will be (i) restarting (ii) modification for convergence (iii) continuation and global convergence (iv) vector vs. scalar labels (v) finding all zeros in the complex domain. Much of the ensuing discussion is informal and selective, with no pretense concerning complete coverage. The motivation is to give a subjective overview of some of the influential past developments, some of the current work, and potential future directions.

2. Restarting. In the first five years of this field considerable attention was focused on the problem of obtaining a satisfactory restart procedure. The initial algorithm of Scarf, when terminated, could not be restarted (using a finer grid) without returning to the original starting point, thereby obviating the possibility of using information obtained the first time through. For the case of vector labelings (both scalar and vector labelings were introduced by Scarf in his 1967 paper) the problem was independently solved by Merrill [29] and Eaves [7]. For the case of scalar labels the problem was independently solved by Fisher, Gould, and Tolle, presented in [9] and [10], and by Kuhn [24] and Kuhn and MacKinnon [25]. It is probably true that most algorithms today use a so-called "sandwich" approach to the restart problem. Briefly, this involves selecting an initial point, x⁰, and then using this point as a base to triangulate the space

 $\mathbb{R}^n \times [0,1]$ (where n is the dimension of the domain and the range of the function f to be studied. The vertices are on the upstairs and downstairs layers $\mathbb{R}^n \times \{0\}$ and $\mathbb{R}^n \times \{1\}$ and the initial simplex contains \mathbf{x}^0 . Each downstairs vertex $\begin{bmatrix} \mathbf{v} \\ 0 \end{bmatrix}$ is given an artificial label according to its relation to an initial starting point $\begin{bmatrix} \mathbf{x}^0 \\ 0 \end{bmatrix} \in \mathbb{R}^n \times \{0\}$. Each upstairs vertex $\begin{bmatrix} \mathbf{v} \\ 1 \end{bmatrix}$ is labeled according to the value of f at v. The grid size is fixed and beginning with the initial simplex a simplicial path is generated by complementary pivoting. If the algorithm terminates (with a complete simplex) then a new starting point $\begin{bmatrix} \mathbf{x}^1 \\ 0 \end{bmatrix}$ in the final complete simplex may be selected, a new triangulation with a finer grid imposed, this time with reference to \mathbf{x}^1 , and the method repeated. In this way each major cycle begins, roughly speaking, where the previous cycle ended. This sandwich method can be used in conjunction with both vector and scalar labels. I will return to this topic in Section 5.

3. Modification for Convergence. It is only in the last 3 or 4 years that convergence properties began to be fairly well understood even at the local level. There is still far to go on the global level. It can be shown that for trivial systems of equations some of the initially proposed algorithms diverged from all starting points, no matter how close to a solution. And yet, with either a new subscripting of the components of f, or by selectively changing some of the f_i to $-f_i$, the same algorithm would converge from any starting point, no matter how far $\frac{3}{}$ from a solution. For example, consider the system

$$f_1(x_1, x_2) = -x_1 + 1$$

$$f_2(x_1, x_2) = x_2 - 1$$

and suppose one attempts to find the trivial root by using either Merrill's vector

 $[\]frac{3}{1}$ In the quasi-Newton context similar benign effects have been noted from a rearrangement of the components of f. See, for example, Broyden [3].

labeling algorithm or any of the original scalar labeling methods. The algorithm will diverge from every starting point. If we multiply f_1 by -1, however, and then apply these same algorithms to solve

$$x_1 - 1 = 0$$

$$x_2 - 1 = 0$$

we observe global convergence.

In early 1974 this orientation problem was clarified by Fisher, Gould, and Tolle [10] under the assumption that f' is nonsingular at a zero, x^* . Under this condition let us define

$$g(x) = (f'(x^0))^{-1} f(x)$$

If it is assumed that x^0 is close to x^* then $(f'(x^0))^{-1}$ exists, and, moreover, the above mentioned algorithms applied to the problem of solving g(x) = 0 will converge to x^* (a root of f and of g). It was thus shown that by modifying the original function f(x) a Newton-like local convergence result is obtained.

At least two prominent problems on convergence remain. Let us first note the perhaps obvious fact that complementary pivoting methods are slow. If a good initial estimate of x* is available then either Newton's method or a quasi-Newton method is to be preferred because of the quadratic convergence properties. For real algebraic equations, however, the domain of convergence of such methods tends to be inversely related to the degree and the number of the equations. Consequently, for highly nonlinear systems it is not surprising

to find a very small domain of convergence. It is precisely when the initial estimate may not be close enough that the slower complementary pivoting methods may be preferable. Thus local convergence results for complementary pivoting fall short of what we are really after--namely, good global results. These are just beginning to appear and will be discussed in the next section.

The second problem alluded to above is that for highly nonlinear systems $f'(x^0)^{-1}$ may be quite expensive or even impossible to obtain analytically. To date there has been little in the way of reported experience on using either discrete approximations or other matrix iterations to replace this term.

4. Continuation and Global Convergence. Continuation methods for solving nonlinear equations date back at least to work of Davidenko in 1953 [5], and have been rediscovered many times since [11], [6], [21], [20], [30], [32], [3], [2]. It now appears that simplicial approximation can be viewed as yet another rediscovery of a continuation method, albeit an especially attractive method—especially attractive because Jacobian singularities do not create the obstacle they do with other such methods. In order to explain some of the recent results in this area, let $H: \mathbb{R}^{n+1} \to \mathbb{R}^n$ be a \mathbb{C}^2 map, let x denote a point in \mathbb{R}^n , t a scalar variable, and suppose H(x, t) has the following homotopy properties:

$$H(x, 0) = f(x), H(x^{0}, 1) = 0$$
 for some known x^{0} .

Two prominent examples are:

- (1) $H(x, t) \equiv f(x) t f(x^0)$ (the Newton homotopy)
- (2) $H(x, t) \equiv t(x x^0) + (1 t) f(x)$ (the Levenberg-Marquardt homotopy) where in either case x^0 is a given initial point in R^n and $t \in [0, 1]$. The

continuation method considers the set of points (x, t) for which

(3) H(x, t) = 0.

Previous works on continuation have generally suffered from the assumption that there exists a continuous solution curve x(t) such that for $t \in [0, 1]$ (x(t), t) is a solution of (3) and that, moreover, $H_{X}(x(t), t)$ is nonsingular for all $t \in [0, 1]$. Under these strong assumptions it follows from the implicit function theorem that x(t) satisfies, for $t \in [0, 1]$,

(4)
$$0 = \frac{d}{dt} H(x(t), t) = H_x \cdot \dot{x} + H_t, \quad x(1) = x^0, \quad \text{or}$$

(5)
$$\dot{\mathbf{x}} = -\mathbf{H}_{\mathbf{x}}^{-1} \mathbf{H}_{\mathbf{t}}, \quad \mathbf{x}(1) = \mathbf{x}^{0}$$

where \dot{x} denotes $\frac{dx}{dt}$. Conversely, if x(t) is a solution of (5) on [0, 1] then, by (4), H(x(t), t) is constant for $t \in [0, 1]$ and $f(x(0)) = H(x(0), 0) = H(x(1), 1) = H(x^0, 1) = 0$. Thus x(0) is a root of f(x). This means that f(x) = 0 can be solved by numerically integrating the differential equation (5) and "continuing" the solution curve x(t) from the known point $x^0 = x(1)$ to the root x(0).

It is not difficult to show that if the differential equation (5) corresponding to the homotopy (1) is integrated by Euler's method then essentially the Newton iterations are obtained [32]. For the differential equation corresponding to the homotopy (2) a variant of the Levenberg-Marquardt method [27], [28], [1] is obtained.

Now we discuss the relations between homotopies and complementary pivoting. It has been known for some time that the set H(x, t) = 0, where H is given by (2), is followed in a limiting sense (piecewise linearly) by Merrill's algorithm.

The set H(x, t) = 0 where H is given by the Newton homotopy (1) has been recently analyzed [15] in detail and it has been shown that (i) the assumption on the existence of a solution curve x(t) can be dropped and (ii) singularities of f'(x) do not cause the usual problems. In particular, let $z = (x, t) \in \mathbb{R}^{n+1}$ and suppose f(x) and hence H(z) given by (1) is c^2 . Let H'(z) denote the $n \times n + 1$ Jacobian matrix $[H_X(z), H_t(z)] = [f'(x), -f(x^0)]$, and suppose rank H' = n for all (x, t) in \mathbb{R}^{n+1} satisfying (3). If this assumption is not satisfied it will be (by Sard's Theorem [35]) for an arbitrarily small perturbation of the right hand side of (3). Hence, for computational purposes the rank n assumption is quite valid. Under these assumptions, the points (x, t) in $H^{-1}(0)$ form a C^1 one-dimensional manifold [31]. Each (connected) component of $H^{-1}(0)$ can therefore be described by a C^1 function $z(\theta) = (x(\theta), t(\theta))$ which is diffeomorphic to a circle or an interval.

Now let $(x(\theta), t(\theta))$ denote the component of $H^{-1}(0)$ containing $(x^0, 1)$ where $x(0) = x^0$, t(0) = 1. Hence $f(x(\theta)) - t(\theta)$ $f(x^0) \equiv 0$. Beginning at x^0 , the projection of this component into R^n can be traced with complementary pivoting on an appropriately labeled triangulation of R^n .

Note that $x(\theta)$, $t(\theta)$ also satisfy the following differential equation:

$$0 = H_{\mathbf{x}} \frac{d\mathbf{x}}{d\theta} + H_{\mathbf{t}} \frac{d\mathbf{t}}{d\theta} = f'(\mathbf{x}(\theta)) \frac{d\mathbf{x}}{d\theta} - f'(\mathbf{x}^{0}) \frac{d\mathbf{t}}{d\theta}$$
$$= f'(\mathbf{x}(\theta)) \frac{d\mathbf{x}}{d\theta} - \frac{f(\mathbf{x}(\theta))}{t(\theta)} \frac{d\mathbf{t}}{d\theta}$$

for $t(\theta) \neq 0$. That is

(6)
$$f'(x(\theta))\dot{x}(\theta) = \frac{\dot{t}(\theta)}{\dot{t}(\theta)} f(x(\theta)), (x(0), t(0)) = (x^{0}, 1), \text{ all } \theta \ni \dot{t}(\theta) \neq 0.$$

This is closely related to an equation studied by Branin [2] and later by Smale [34]. The following recent path theorem [14] shows that $\dot{t}(\theta) = 0 \iff \det f'(x(\theta)) = 0$. Hence, for $\dot{t}(\theta) \neq 0$, $f'(x(\theta))^{-1}$ exists, and for such values of θ , provided $t(\theta) \neq 0$, $\dot{x}(\theta)$ in (6) is always either in the Newton direction or the negative of the Newton direction, depending on the sign of $\dot{t}(\theta)/t(\theta)$.

A Path Theorem:

Let $H: \mathbb{R}^{n+1} \to \mathbb{R}^n$ be \mathbb{C}^2 and 0 a regular value of H (i.e., H'(z) has rank $n \ \forall \ z \in H^{-1}(0)$). Then for any component $z(\theta)$ of $H^{-1}(0)$ we have for $i = 1, \ldots, n+1$

$$\operatorname{sgn} \dot{z}_{i}(\theta) = \operatorname{sgn} \det H^{i}(x(\theta)), \text{ all } \theta$$

or

$$\operatorname{sgn} \dot{z}_{i}(\theta) = -\operatorname{sgn} \det H^{i}(x(\theta)), \text{ all } \theta$$

where sgn $0 \stackrel{\Delta}{=} 0$, and Hⁱ denotes all columns of H' but the ith.

For the Newton homotopy this theorem implies

$$sgn \ t(\theta) = sgn \ det \ f'(x(\theta)), \ all \ \theta$$

$$or$$

$$sgn \ t(\theta) = -sgn \ det \ f'(x(\theta)), \ all \ \theta$$

Also, from the above path theorem, it is clear that for the Newton homotopy $t(\theta)$ is strictly monotonic (and hence invertible to obtain $\theta(t)$) on a particular

component of $H^{-1}(0)$ iff $f'(x(\theta))$ is nonsingular on that component and hence only under this condition can $x(\theta)$ be expressed as a function of t (i.e., $x(\theta(t))$, and even so it need not be true that t varies between 0 and 1 on this component. On the other hand, if f' has a singularity on a component then it cannot be expected that x will be a function of t on that component and the usual continuation methods will most likely encounter difficulty. Such a singularity should not be considered particularly pathological. As an illustration consider the following simple example due to Freudenstein and Roth [11].

$$f_1(x_1, x_2) = -13 + x_1 - 2x_2 + 5x_2^2 - x_2^3 = 0$$

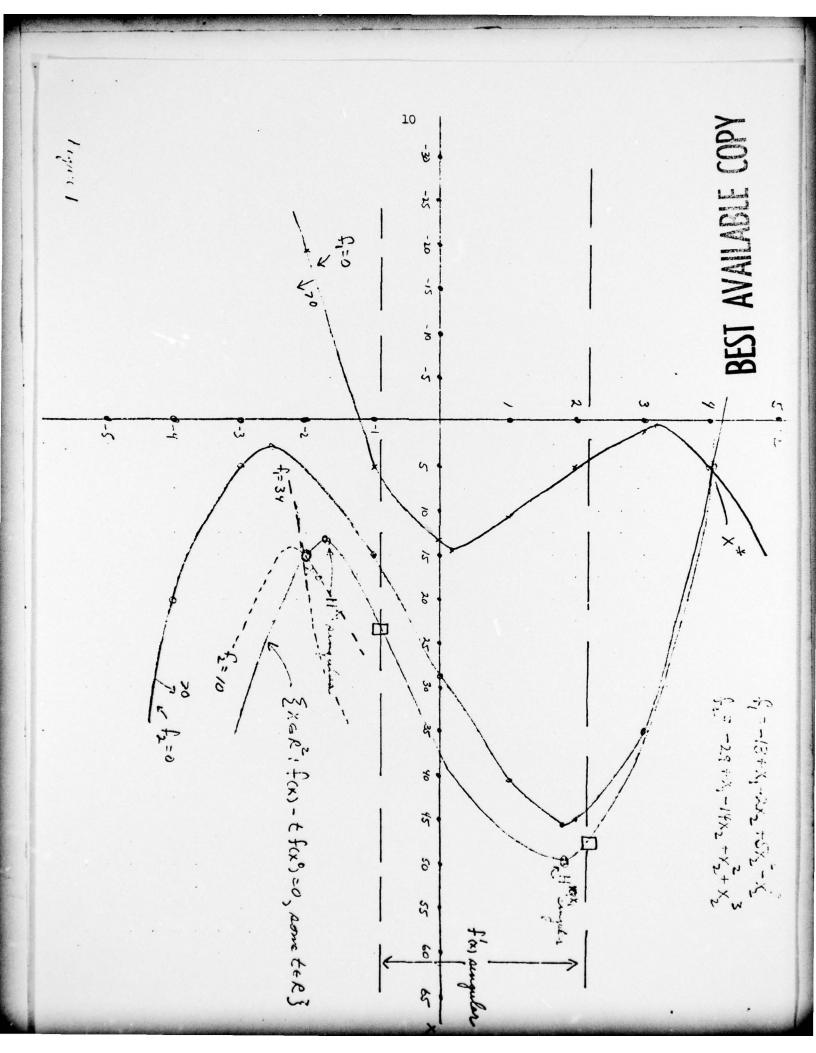
 $f_2(x_1, x_2) = -29 + x_1 - 14x_2 + x_2^2 + x_2^3 = 0$.

Here, letting H(x, t) be given by (1), and taking $x^0 = (15, -2)$, we obtain

$$H'(x, t) = \begin{bmatrix} 1 & -2 + 10x_2 - 3x_2^2 & -34 \\ 1 & -14 + 2x_2 + 3x_2^2 & -10 \end{bmatrix} = [f'(x), -f(x^0)] .$$

It can be easily verified that $H^t = f'(x)$ is singular whenever $x_2 = 2.23$ or $x_2 = -.897$. In Figure 1 it is seen that the path H(x, t) = 0 crosses each of these lines. Both Newton's method and Broyden's quasi-Newton continuation method have been reported to fail (starting at $x^0 = (15, -2)$) on this example. The simplicial approximation G^2 algorithm [13], [15] can be shown to converge to the unique root at (5.0, 4.0).

In order to illustrate the application of complementary pivoting and simplicial approximation let us focus on the Newton homotopy



(7)
$$H(x, t) = f(x) - t f(x^0) = 0, x \in \mathbb{R}^n, t \in \mathbb{R}$$
.

It is important to note in (7) that t is not confined to [0, 1]. In particular, beginning at x^0 , t may well become greater than 1 on the homotopy path $z(\theta)$ before encountering the value zero (at which time a root of f is at hand). For H as given by (7), the projection into R^n of the component of $H^{-1}(0)$ containing the point x^0 can be tracked in a precise limiting sense by the Garcia Gould algorithm discussed in [15] and [13]. The algorithm is always initiated with $\theta = 0$ at $x(0) = x^0$ such that $\det f'(x^0) \neq 0$, and t(0) = 1. Also we always move initially in such a way that $\dot{t}(0) < 0$. This means that the initial direction is always Newton (since $\frac{\dot{t}(0)}{t(0)} < 0$ in expression (6)). The negativity of $\dot{t}(0)$, along with the path theorem, also implies

det
$$f'(x^0) > 0 \Rightarrow sgn \dot{t}(\theta) = -sgn \det f'(x(\theta))$$
, all θ
det $f'(x^0) < 0 \Rightarrow sgn \dot{t}(\theta) = sgn \det f'(x(\theta))$, all θ .

Thus, for all $\theta \ni t(\theta) > 0$,

$$\det \ f'(x^0) > 0 \Rightarrow \dot{x}(\theta) \quad \text{is Newton} \iff \det \ f'(x(\theta)) > 0$$

$$\det \ f'(x^0) < 0 \Rightarrow \dot{x}(\theta) \quad \text{is Newton} \iff \det \ f'(x(\theta)) < 0 \quad .$$

Concerning convergence, the following interesting global result is initially due to Smale [34]:

Suppose there is an open bounded set C such that $f \colon \overline{C} \to \mathbb{R}^n$, C and ∂C are connected, \mathcal{X} smooth, and $x \in \mathcal{X} \Longrightarrow \det f'(x) > 0$ and $f'(x)^{-1} f(x)$ intersects \mathcal{X} transversally at x. Suppose $f \in C^2$, $x^0 \in \mathcal{X}$, and rank H'(x, t) = n

for all (x, t) in $H^{-1}(0)$. Then the projection into \mathbb{R}^n of the connected component of $H^{-1}(0)$ containing $(x^0, 1)$ will contain a zero of f.

Although the conditions of this theorem are weak (nonsingularity of f'(x) on $x(\theta)$ is not assumed) it is clear from the simple example in Figure 1 that they are still too strong. It can be seen in this figure that if $x^0 \in \mathcal{X}$, for any open bounded connected C containing x^* , then \mathcal{X} will contain 4 points at which det f' = 0. In fact, a necessary and sufficient condition for the G^2 algorithm to encounter a regular zero (at which det $f' \neq 0$) is:

There exists a point $(\hat{x}(\hat{\theta}), \hat{t}(\hat{\theta}))$ on the path $(x(\theta), t(\theta))$ such that

(i) sgn det $f'(x^0) = \text{sgn det } f'(\hat{x})$ i.e., det f'(x) changes sign an even number of times between x^0 and \hat{x} .

(ii) $\dot{x}(\dot{\theta})$ is the negative of the Newton direction. The sufficiency is proved by observing that

$$1 = \operatorname{sgn}\left(\frac{\dot{t}(\hat{\theta})}{\dot{t}(\hat{\theta})}\right) = \frac{\operatorname{sgn}\dot{t}(0)}{\operatorname{sgn}\dot{t}(\hat{\theta})} = \frac{-1}{\operatorname{sgn}\dot{t}(\hat{\theta})} \Rightarrow \operatorname{sgn}\dot{t}(\hat{\theta}) = -1.$$

The necessity can be seen by noting that the sign of $\dot{x}(\theta)$ reverses each time $\dot{t}(\theta)/t(\theta)$ changes sign. Letting $\overline{\theta}$ be the first θ value such that $f(x(\overline{\theta})) = 0$, the sign of $t(\theta)$ at $\overline{\theta} + \varepsilon$, for small ε , will have undergone one reversal $(\dot{t}(\overline{\theta}) \neq 0$ since det $f'(x(\overline{\theta})) \neq 0$). By the Newton-Kantorovich Theorem $\dot{x}(\overline{\theta} + \varepsilon)$ has the negative Newton direction. Hence $\dot{t}(\theta)$ and therefore det f' has reversed sign an even number of times. Examples of this result are

illustrated in Figures 2 and 3.

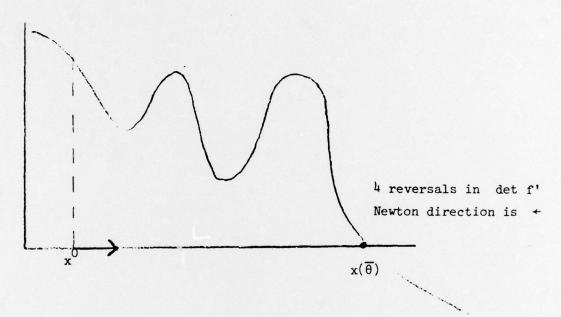
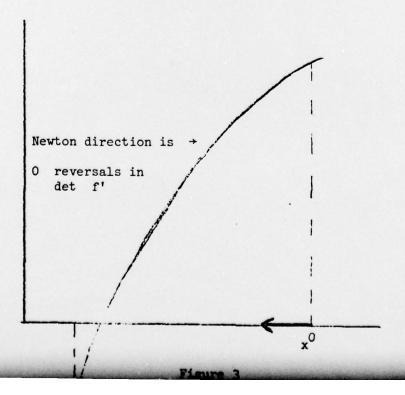


Figure 2



In concluding this section we make note of several additional convergence properties. Suppose the component of $H^{-1}(0)$ containing $(x^0, 1)$ is an 'unbounded path. Assume that on this path \dot{x} eventually has the negative of the Newton direction. Also assume that det $f'(x) \neq 0$ if $x \in f^{-1}(0)$ (so that a zero corresponds to a change in sign of t). Then we have the opposite parity result:

reversals in det f' is even (odd) \iff # zeros on path is odd(even). This is proved by noting that an even (odd) number of reversals in det f' (i.e., in t) gives an even (odd) number of reversals in the sign of x . Since x is initially in the Newton direction, and eventually in the negative of the Newton direction, an even (odd) number of reversals in det f' implies an odd (even) number of reversals in t (= # zeros).

From this opposite parity result it follows that an unbounded path must contain either a zero or an odd number of reversals in det f'. Note that any path in R¹ is unbounded and this result applies (c.f. Figures 2 and 3).

If the component of $H^{-1}(0)$ containing $(x^0, 1)$ is a <u>loop</u> (n must be > 1), there must be an even number of reversals in det f' and an even number of zeros. This follows from the fact that $\dot{t}(1) = \dot{t}(0) < 0$ and hence the reversals in det f' are even in number. Also, since \dot{x} is continuous and $\dot{x}(0) \neq 0$, there must be an even number of reversals in \dot{t}/t and, since even in \dot{t} , also even in t.

From these comments it follows that if there is a unique zero then it lies on an unbounded path with an even number of reversals in det f'. This case is illustrated in Figure 1.

As a final comment, examples can be found for which solving Smale's equation, or using G² on the Newton homotopy (7) (which has an advantage that many roots can possibly be located) has the interesting property that convergence occurs when starting far away, or, as usual, from very close, but not from intermediate points. Also, it is not yet clear what classes of functions satisfy the above discussed convergence conditions. Thus, from the viewpoint of global convergence, these continuation-like methods leave many important questions to be answered.

- 5. <u>Vector versus Scalar Labels</u>. Another area under active pursuit involves the question of relative efficiency between vector and scalar labels. The vector labeling procedure requires the solution of a linear system at each iteration (each time a vertex is eliminated). In the sandwich method, then, for tracking, for example,
- (8) $H(x, t) \equiv t(x x^0) + (1 t) f(x) = 0$, $x \in \mathbb{R}^n$, $t \in [0, 1]$ with vector labels an order of $(n + 1)^2$ multiplications are required per pivot. It has recently been demonstrated that each of the homotopies (7) and (8) can be tracked with scalar labels, and, moreover, a sandwich is not required [12], [13]. Thus, only an order of n multiplications per pivot is required. Considering a given homotopy, such as (7) for example, we then have the result that precisely the same path, in a limiting sense, is followed by either a vector or a scalar labeling. However, this does not imply that the simplicial paths will be identical for these two procedures. Herb Scarf has conjectured that, for example, the scalar path will "wiggle" more than the vector path, for the vector path enjoys the property that on each simplex a piecewise linear approximation to H(x, t) = 0 is obtained. However, even if the scalar path would require

more iterations (and this is not yet clear), it would remain to determine which method on net involves more computational work.

Indeed there are other scalar labeling methods which were proposed in the early 1970's. Limited evidence suggests that these earlier methods are not as effective as the vector methods, at least via the sandwich approach, but it would seem to be of interest to explore such methods in conjunction with a full triangulation of $\mathbb{R}^n \times [0, 1]$, i.e., triangulate the $n + 1^{st}$ dimension as well as \mathbb{R}^n . One could then apply scalar labels to $\mathbb{H}(x, t)$ and this would provide yet another means for tracking $\mathbb{H}(x, t) = 0$, beginning on $\mathbb{R}^n \times \{1\}$.

6. Finding All Zeros in the Complex Domain. Perhaps the most exciting recent work in the field is due to Garcia and Zangwill [16], [17] and gives, for the first time, a systematic and fail-safe method for finding all roots of certain systems of n equations in n complex variables. The work applies to arbitrary polynomials and even more general systems. The approach presented goes roughly as follows. One wishes to solve

$$P_{j}(z) = 0, j = 1, ..., n$$

where each P_j : $C^n \to C$ is analytic and P(z) = 0 has a bounded solution set. The system

(9)
$$(1-t) Q_j(z) + t P_j(z) = 0, j = 1, ..., n (t \in R)$$

is considered, where

(a) the set of solutions to the "simple system" Q(z) = 0 is bounded and known

(b) if
$$||z|| \to \infty$$
 then, for some j, $\lim_{z \to 0} \frac{P_j(z)}{Q_j(z)}$, if real, is not negative.

Each known solution at t=0 serves as a starting point. The simplicial path will either diverge to infinity as t+1 or will terminate at t=1.

Moreover, each path starting from a solution to $P_j(z)=0$ (at t=1) will link to t=0. This is subject to the assumption that 0 is a regular value of (9), which is satisfied with probability one. The above properties imply that all roots of P(z)=0 will be hit by a subset of the paths leading from the known solutions (at t=0) to Q(z)=0. This work has obvious and important implications for global optimization where the optimum optimorium of a nonconvex (or noncave) differentiable function is sought.

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